Advanced Research Center for Beam Science
– Atomic and Molecular Structures –

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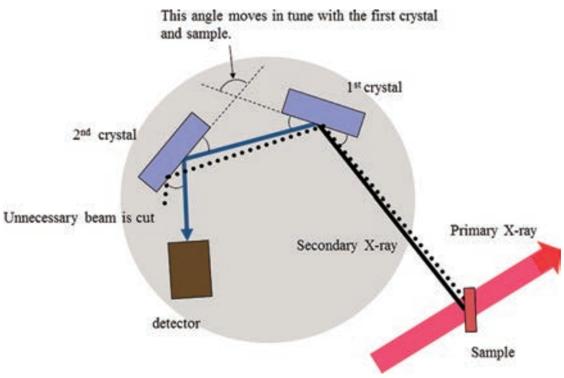
Scope of Research

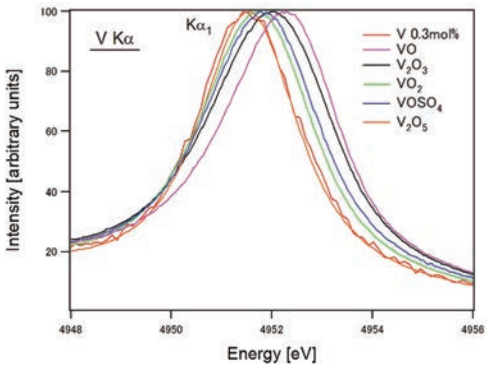
Our laboratory analyzes the electronic state of atomic or molecular structure in materials, which are obtained from diffraction and spectra observed by X-ray irradiation, respectively, to elucidate the relationships between the structure and the physical properties. Our main themes are (1) high-resolution experimental and theoretical studies on the natural linewidth of elements in materials, (2) the development of the spectrometer in the measurements of the diagram lines in soft X-rays region, and (3) structural determination of novel protein molecules and their complexes.

KEYWORDS

High Resolution X-ray Crystal Spectrometer
Natural Linewidth
Chemical Shift
Structural Biology
Protein Crystallography



Oxidation state on V and Mn $K\alpha_1$ x-ray emission spectra



Selected Publications

Ito, Y.; Tochio, A.; Vlaicu, H.; Yamashita, M.; Fukushima, S.; Polasik, M.; Slabkowska, K.; Syrocki, L.; Szymanska, E.; Rzadkiewicz, J.; Indelicato, P.; Marques, J. P.; Martins, M. C.; Santos, J. P.; Parente, F., Structure of High-resolution $K\beta_{1,3}$ X-Ray Emission Spectra for the Elements from Ca to Ge, *Phys. Rev.*, **A97,** [052505-1]-[052505-10] (2018).

Menesguen, Y.; Lepy, M.-C.; Honicke, P.; Muller, M.; Unterumsberger, R.; Beckoff, B.; Hoszowska, J.; Dousse, J.-Cl.; Blachucki, W.; Ito, Y.; Yamashita, M.; Fukushima, S., Experimental Determination of X-Ray Atomic Fundamental Parameters of Nickel, *Metrologia*, **55,** 56 (2018).

Tanikawa, T.; Ito, Y.; Fukushima, S.; Yamashita, M.; Sugiyama, A.; Mizoguchi, T.; Okamoto, T.; Hirano, Y., Calcium Is Cycled Tightly in *Cryptomeria Japonica* Stands on Soils with Low Acid Buffering Capacity, *For. Ecol. Manage.*, **399,** 64-73 (2017).

Ito, Y.; Tochio, T.; Ohashi, H.; Yamashita, M.; Fukushima, S.; Polasik, M.; Slabkowska, K.; Syrocki, L.; Szymanska, E.; Rzadkiewicz, J.; Indelicato, P.; Marques, J. P.; Martins, M. C.; Santos, J. P.; Parente, F., $K\alpha_{1,2}$ X-ray Linewidths, Asymmetry Indecies, and [*KM*] Shake Probabilities in Elements Ca to Ge and Comparison with Theory for Ca, Ti, and Ge, *Phys. Rev.*, **A94,** [42506-1]-[42506-11] (2016).

Fujii, T.; Sato, A.; Okamoto, Y.; Yamauchi, T.; Kato, S.; Yoshida, M.; Oikawa, T.; Hata, Y., The Crystal Structure of Maleylacetate Reductase from *Rhizobium* sp. Strain MTP-10005 Provides Insights into the Reaction Mechanism of Enzymes in Its Original Family, *Proteins: Structure, Function, and Bioinformatics*, **84,** 1029-1042 (2016).

Fujii, T.; Yamauchi, T.; Ishiyama, M.; Gogami, Y.; Oikawa, T.; Hata, Y., Crystallographic Studies of Aspartate Racemase from *Lactobacillus sakei* NBRC 15893, *Acta Crystallogr. Sect. F Struct. Biol. Cryst. Commun.*, **71,** 1012-1016 (2015).

The Spin Doublets, FWHM, and Shake Probabilities in 3d $K\beta_{1,3}$ Spectra

The content described below is another result of our research on the spin doublets and the asymmetry of the $K\beta_{1,3}$ x-ray emission spectra in the 3*d* transition metals that has been unknown in the history of about 100 years in Atomic Physics.

The $K\beta_{1,3}$ x-ray emission spectra include $K\beta$' and $K\beta$" satellites on the low- and high-energy side of the $K\beta_{1,3}$ peak position, respectively, as explained in the case of copper. These satellites have also been investigated until now both experimentally and theoretically for all 3*d* transition metals. Shake-up from the 3*d* shell was also shown to account reasonably well for the measured $K\beta_{1,3}$ line shape, although a complete quantitative fitting has not been reported and possible contributions from other shells were not investigated. The low-energy satellite group, denoted by $K\beta$', received special attention, and several other sources such as exchange interaction and plasmon oscillations were suggested as its origin. It has been assumed that the line shape can be fully accounted for by satellites resulting from 3*l* spectator holes in addition to the nominal single-electron diagram transitions.

We have investigated the $K\beta_{1,3}$ x-ray spectra of the elements from Ca to Ge using a high-resolution antiparallel double-crystal x-ray spectrometer (Figure 1). Each $K\beta_{1,3}$ natural line width has been corrected using the instrumental function of this type of x-ray spectrometer, and the spin doublet energies have been obtained from the peak position values in $K\beta_{1,3}$ x-ray spectra (Figure 2). Moreover, it has been found that the contribution of satellite lines are considered to be [*KM*] shake processes (Figure 3).

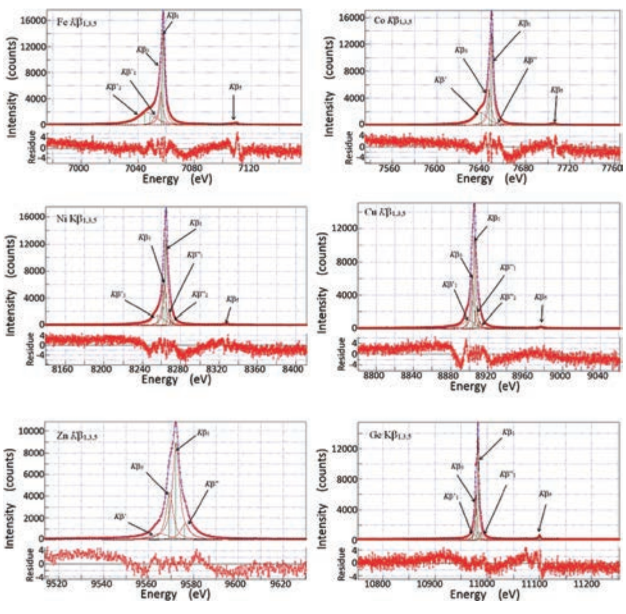


Figure 1. The observed $K\beta_{1,3}$ spectra in elements Fe to Ge are shown with the fitting Lorentzian function (Phys Rev A97, 052505). These spectra were measured using the antiparallel double-crystal x-ray spectrometer described in detail in Phys Rev A94,042506. In this figure, the $K\beta$" line is a satellite line resulting from a 3*d* spectator hole.

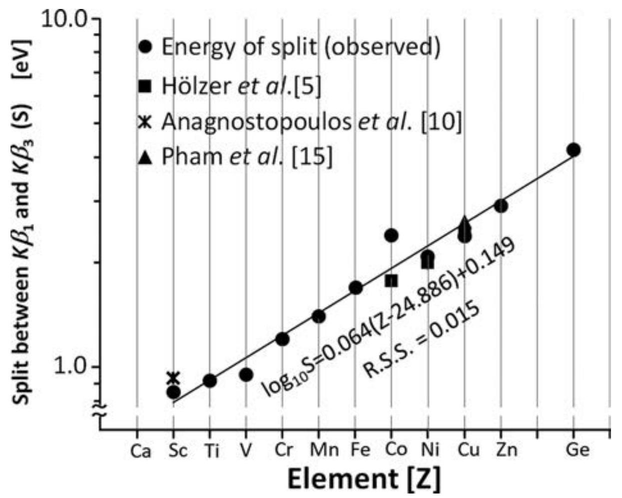


Figure 2. The spin doublet energies of $K\beta_1$ and $K\beta_3$ lines for elements Sc to Ge. The least-squares fitting was executed using data in the present work.

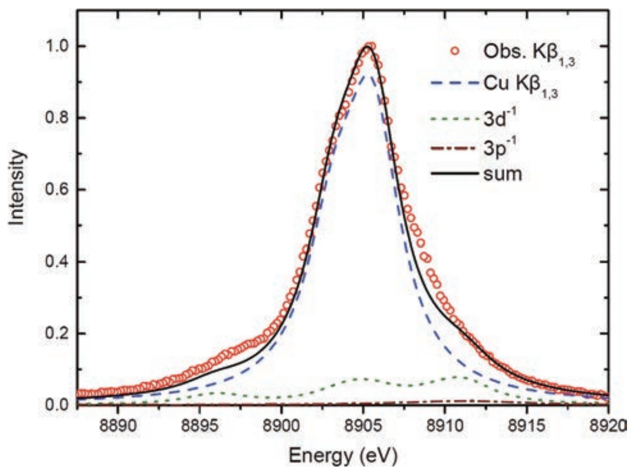


Figure 3. Comparison of the high-resolution experimental spectra with the predicted $K\beta_{1,3}$ spectra of Cu including the contributions of the $K\beta_{1,3}$ diagram lines and the satellite lines for [1s3p] and [1s3*d*] hole states.